

Chapter 2

An Introduction to Organic Compounds

Hydrocarbons, Backbone, Functions, Nomenclature, Physical Properties, and Conformations

Adapted from Turro & Breslow, Columbia University and Irene Lee, Case Western Reserve University

HYDROCARBONS

- Compounds composed of only carbon and hydrogen atoms (C, H). Each carbon has 4 bonds.
- They represent a "backbone" when other "heteroatoms" (O, N, S,) are substituted for H. (The heteroatoms give function to the molecule.)
- Acyclic (without rings); Cyclic (with rings); Saturated: only carbon-carbon single bonds; Unsaturated: contains one or more carbon-carbon double and/or triple bond

HYDROCARBONS

- Alkanes contain only single (σ) bonds and have the generic molecular formula: $[C_nH_{2n+2}]$
- Alkenes also contain double ($\sigma + \pi$) bonds and have the generic molecular formula: $[C_nH_{2n}]$
- Alkynes contain triple ($\sigma + 2\pi$) bonds and have the generic molecular formula: $[C_nH_{2n-2}]$
- Aromatics are planar, ring structures with alternating single and double bonds: eg. C_6H_6

Types of Hydrocarbons



Each C atom is tetrahedral with sp^3 hybridized orbitals. They only have single bonds.



Each C atom is trigonal planar with sp^2 hybridized orbitals. There is no rotation about the C=C bond in alkenes.

Types of Hydrocarbons

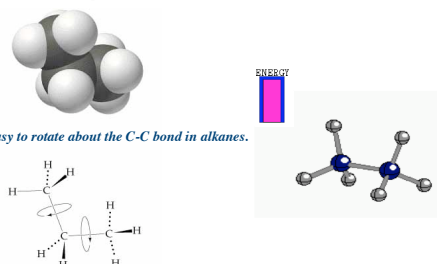


Each C atom is linear with sp hybridized orbitals.



Each C-C bond is the same length; shorter than a C-C bond; longer than a C=C bond. The concept of resonance is used to explain this phenomena.

Propane



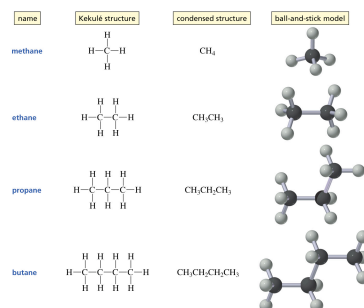
Naming Alkanes

$C_1 - C_{10}$: the number of C atoms present in the chain.

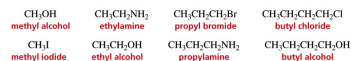
FIRST SEVERAL MEMBERS OF THE STRAIGHT-CHAIN ALKANE SERIES

| Molecular Formula | Condensed Structural Formula | Name | Boiling Point (°C) |
|-------------------|--|---------|--------------------|
| CH_4 | CH_4 | Methane | -216.1 |
| C_2H_6 | CH_3CH_3 | Ethane | -289 |
| C_3H_8 | $CH_3CH_2CH_3$ | Propane | -244 |
| C_4H_{10} | $CH_3CH_2CH_2CH_3$ | Butane | -20.5 |
| C_5H_{12} | $CH_3CH_2CH_2CH_2CH_3$ | Pentane | 36 |
| C_6H_{14} | $CH_3CH_2CH_2CH_2CH_2CH_3$ | Hexane | 68 |
| C_7H_{16} | $CH_3CH_2CH_2CH_2CH_2CH_2CH_3$ | Heptane | 98 |
| C_8H_{18} | $CH_3CH_2CH_2CH_2CH_2CH_2CH_2CH_3$ | Octane | 125 |
| C_9H_{20} | $CH_3CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_3$ | Nonane | 151 |
| $C_{10}H_{22}$ | $CH_3CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_3$ | Decane | 174 |

Each member $C_3 - C_{10}$ differs by one CH_2 unit. This is called a *homologous series*.
Methane to butane are gases at normal pressures.
Pentane to decane are liquids at normal pressures.



Nomenclature of Alkyl Substituents



- Constitutional or structural isomers have the same molecular formula, but their atoms are linked differently
- Naming has to account for them.

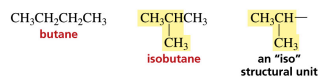
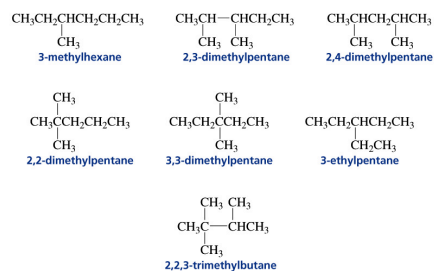


Table 2.2 Names of Some Alkyl Groups

| | | | |
|-----------|-------------------------|------------|-----------------------------------|
| isobutyl | $CH_3CH_2CH_2-$ | sec-butyl | CH_3CH_2CH- CH_3 |
| isopentyl | $CH_3CH_2CH_2CH_2-$ | tert-butyl | CH_3 CH_3C- CH_3 |
| isopentyl | $CH_3CH_2CH_2CH_2-$ | isopentyl | $CH_3CH_2CH_2CH_2CH_2-$ CH_3 |
| isobutyl | CH_3CHCH_2- CH_3 | isopentyl | $CH_3CHCH_2CH_2-$ CH_3 |

- A compound can have more than one name, but a name must unambiguously specify only one compound

A C_7H_{16} compound can be any one of the following:

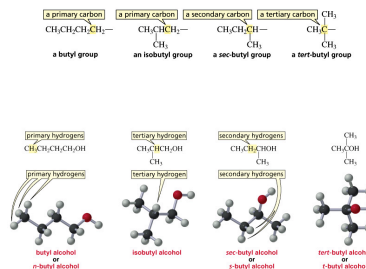


Alkanes

(Different types of sp^3 carbon atoms)

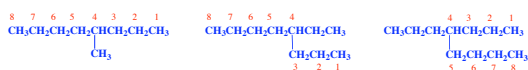
- **Primary, 1°** , a carbon atom with 3 hydrogen atoms: $[R-CH_3]$
- **Secondary, 2°** , a carbon atom with 2 hydrogen atoms: $[R-CH_2-R]$
- **Tertiary, 3°** , a carbon atom with 1 hydrogen atom: $[R-\underset{\text{H}}{\underset{|}{\text{C}}}-R]$
- **Quaternary, 4°** , a carbon atom with 0 hydrogen atoms: CR_4

Different Kinds of sp^3 Carbons and Hydrogens

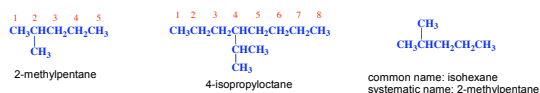


Nomenclature of Alkanes

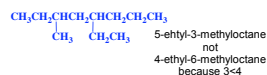
- Determine the number of carbons in the parent hydrocarbon



- Number the chain so that the substituent gets the lowest possible number

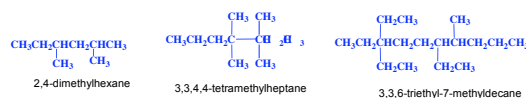


- Number the substituents to yield the lowest possible number in the number of the compound

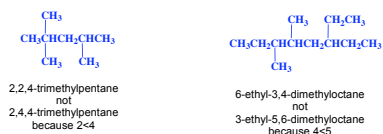


(substituents are listed in alphabetical order)

- Assign the lowest possible numbers to all of the substituents



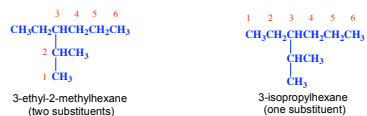
- When both directions lead to the same lowest number for one of the substituents, the direction is chosen that gives the lowest possible number to one of the remaining substituents



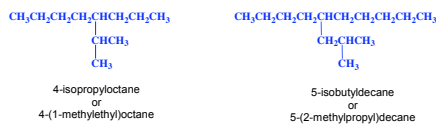
- If the same number is obtained in both directions, the first group receives the lowest number



- In the case of two hydrocarbon chains with the same number of carbons, choose the one with the most substituents



- Certain common nomenclatures are used in the IUPAC system



Click "Next" to view the systematic naming of a hydrocarbon.

$$\begin{array}{c}
 \text{CH}_3\text{CH}_2\text{CH}_2\text{CHCH}_2\text{CH}_3 \\
 | \\
 \text{CH}_2\text{CHCH}_3 \\
 | \\
 \text{CH}_3
 \end{array}$$


Rules Next

C_nH_{2n}


Cycloalkane Nomenclature

Cycloalkanes

- Cycloalkanes are alkanes that contain a ring of three or more carbons.
- Count the number of carbons in the ring, and add the prefix *cyclo* to the IUPAC name of the unbranched alkane that has that number of carbons.



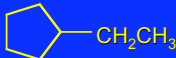
Cyclopentane



Cyclohexane

Cycloalkanes

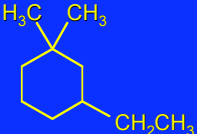
- Name any alkyl groups on the ring in the usual way. A number is not needed for a single substituent.



Ethylcyclopentane

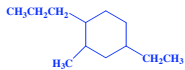
Cycloalkanes

- Name any alkyl groups on the ring in the usual way. A number is not needed for a single substituent.
- List substituents in alphabetical order and count in the direction that gives the lowest numerical locant at the first point of difference.




3-Ethyl-1,1-dimethylcyclohexane

For more than two substituents,



4-ethyl-2-methyl-1-propylcyclohexane
not
1-ethyl-3-methyl-4-propylcyclohexane
because 2 < 3
not
5-ethyl-1-methyl-2-propylcyclohexane
because 4 < 5



1,1,2-trimethylcyclopentane
not
1,2,2-trimethylcyclopentane
because 1 < 2
not
1,1,5-trimethylcyclopentane
because 2 < 5